

Micro-Structures of Opposed
Flow Diffusion Flames: Methane

by

Antonio M. Vincitore(1), Nick M. Marinov(2), William J. Pitz(3),
Charles K. Westbrook(2), Carl F. Melius(3), and Selim M. Senkan(1)

(1) Department of Chemical Engineering
University of California
Los Angeles, CA 90095

(2) Lawrence Livermore National Laboratory
Livermore, CA 94551

(3) Combustion Research Facility
Sandia National Laboratories
Livermore, CA 94551

Abstract

The micro-structure of an opposed flow, methane diffusion flame has been determined using heated micro-probe sampling followed by gas analysis by on-line gas chromatography/mass spectrometry (GC/MS). Mole fraction profiles of major products as well as trace aromatic, and polycyclic aromatic, substituted aromatic hydrocarbons (PAH up to C₁₆H₁₀, e.g. pyrene) were quantified by direct analysis of samples withdrawn from within the flame without any pre-concentration. Mole fractions range from 0.8 to 1.0E-7. The experimental results are compared to results from a newly-developed chemical kinetic model that includes chemistry for the production and consumption of aromatics and PAH species. The model makes reasonable predictions for the major intermediate species profiles and for the peak concentrations of many of the trace aromatics and PAH species.

This work was performed under the auspices of the U.S. Dept. of Energy at LLNL under contract no. W-7405-Eng-48.